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ABSTRACT

The equations implicit in Néel's molecular-field theory of ferrimagnetism are set out in considerable detail. The general equations which pertain to magnetic structures with crystallographic long-range order are derived, and the specific pair of transcendental equations which must be satisfied in the case of two sets of antiparallel magnetic spins is written down in a form which is amenable to solution by automatic computer methods. The dominant interaction is expressed in terms of the magnetic transition temperature, while the two smaller interactions are given as fractions of the dominant one. A computation of the shapes of the curves of the magnetization as a function of temperature shows that, while magnetic and neutron diffraction measurements can determine quite precisely the value of a linear function of these fractions, the actual values of the individual fractions are less precisely determined. It follows that any experimental deviation from the calculated curves is due to an inadequacy of the theory rather than to incorrect values of the parameters. Finally, methods of attack for computation of more complex cases are discussed.

PROBLEM STATUS

This is an interim report on the problem; work is continuing.

AUTHORIZATION

CALCULATION OF MAGNETIZATION VS TEMPERATURE CURVES
FOR FERRIMAGNETIC MATERIALS

INTRODUCTION

The Néel theory of ferrimagnetism (1,2) is recognized universally as providing a good basis for understanding the magnetic properties of a wide variety of substances which contain magnetic ions on two or more crystallographically distinct sets of sites in their crystal structure. The theory basically assumes that it is possible to describe the total magnetic energy of the crystal by an expression of the type

$$E = -\sum J_{ij} \, S_i \cdot S_j \, , \tag{1}$$

where the summation is taken over all pairs of ions i and j, and S_i and S_j are the angular momentum vectors of the ith and jth atoms respectively. The quantity J_{ij} is the exchange integral, which is a measure of the strength of the interaction tending to align the angular momenta of the two ions. If J_{ij} is positive, the energy will be lowest if S_i and S_j are parallel to one another, and, conversely, a negative value of J_{ij} favors antiparallel alignment of S_i and S_j. Under the assumption of Eq. (1) the contribution to the total energy due to the ith ion alone has the same dependence on the angular orientation of S_i as it would have if the ion were a magnetic dipole acted upon by a magnetic field. Equation (1) can then be written in the form

$$E = -\sum_i S_i \cdot \left(\sum_{j \neq i} H_{ij} \right) \tag{2}$$

and the summation over j is termed the "molecular field" acting on the ith ion.

In most crystals we may assume that it is possible to divide each set of crystallographic sites into a finite number of subsets in each of which the time-averaged spin directions are all parallel, and we also assume that the individual contributions to the molecular field are proportional to the expectation values of gS_j, where g is the gyromagnetic ratio. Now

$$g \sum_j S_j$$

is defined as M_j, the magnetization of the set of ions over which the sum has been taken. Therefore, we may express the molecular field acting on the ith ion, or on any other ion in the same subset in the form

$$H_i = \sum_j \alpha_{ij} M_j \, . \tag{3}$$

The coefficients α_{ij} are the "molecular field coefficients" for the interaction ij. The values of these coefficients determine the shapes of the curves of the magnetizations $|M_j|$ as a function of temperature. These individual magnetizations are often called the "sublattice magnetizations," although the sets of crystallographic sites are often not lattices. These curves can be measured by means of neutron diffraction, and sometimes by other

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methods, and, at least in principle, the values of the molecular field coefficients, and therefore an approximation to the values of the exchange integrals, can be inferred from the shapes of the measured curves.

The purpose of this report is to derive the mathematical expressions for these curves in a form amenable to computation, to set down the specific equations which apply to the simple case of two sets of ions with their magnetic moments aligned antiparallel to one another, to describe the results of calculations made using these equations, and to indicate the possible procedures in extending the calculations to more complex situations. The appendix describes in detail a program written for the NAREC computer to do the calculations in the two-set case.

GENERAL EXPRESSIONS FOR THE MAGNETIZATION
VS TEMPERATURE CURVES

It can be shown (3) that an ion in a magnetic field H will have an expected value of its magnetization given by $M = g S \mu_B B_S(x)$, where g is the gyromagnetic ratio, μ_B is the Bohr magneton, and $B_S(x)$ is the Brillouin function,

$$B_S(x) = \frac{2S + 1}{2S} \operatorname{ctnh}\left[\frac{(2S + 1)x}{2S}\right] - \frac{1}{2S} \operatorname{ctnh}\left(\frac{x}{2S}\right), \tag{4}$$

where $x = g S |H| \mu_B / kT$ and S denotes the magnitude of the vector S. The molecular field approach assumes that the same expression can be used if H, instead of being an applied field, is the fictitious "molecular field."

We shall resolve the system of vector equations (3) into sets of three scalar equations involving components along three suitable, orthogonal directions, which will be designated by a running subscript k. Thus,

$$H_{ik} = \sum_j \alpha_{ij} M_{jk}. \tag{5}$$

If we denote the direction cosines of the molecular field H_i by C_{ik}, and remember that M_i is parallel to H_i, Eqs. (5) become

$$|H_i| C_{ik} = \sum_j \alpha_{ij} |M_j| C_{jk}. \tag{6}$$

But $|H_i| = kT x_i / g_i S_i \mu_B$, and $|M_i| = n_i g_i S_i \mu_B B_{Si}(x_i)$, where n_i is the number of ions per formula unit in the ith set. Therefore,

$$kT x_i C_{ik} = \mu_B^2 g_i S_i \sum_j \alpha_{ij} C_{jk} g_j S_j n_j B_{Sj}(x_j). \tag{7}$$

If there are n sets of ion sites, there will be $3n$ equations like (7). A spontaneous magnetic moment can exist if there exists a nonzero vector x with components $x_i C_{ik}$ which is a solution of Eqs. (7), subject, of course, to the restriction that

$$\sum_k C_{ik}^2 = 1. $$

We shall prove later that, in certain special cases at least, a nonzero solution is possible below a certain limiting temperature, which can be identified with the Curie temperature, T_c. Further, we can infer from the laws of thermodynamics that if at least one of

the interactions α_{ij} is nonzero for each value of i (or j) there must be a solution for very small values of T, and this solution must approach $x_i = \infty$ for all values of i as T approaches zero.

THE CASE OF TWO SETS OF IONS

The special case in which the magnetic structure consists of only two sets of magnetic ions oriented antiparallel to one another, with a net moment resulting from either unequal numbers of ions or unequal magnetic moments per ion on the two sets of sites, is of considerable practical importance, as well as mathematically tractable. In this case we can take one of the component directions parallel to the moments, so that $C_{11} = 1$, $C_{21} = -1$, $C_{12} = C_{13} = 0$. Then Eqs. (7) reduce to two only:

$$kTx_1 = \mu_B^2 g_1 S_1 \left[n_1 \alpha_{11} g_1 S_1 B_{S1}(x_1) - n_2 \alpha_{12} g_2 S_2 B_{S2}(x_2) \right] \tag{8a}$$

$$-kTx_2 = \mu_B^2 g_2 S_2 \left[n_1 \alpha_{12} g_1 S_1 B_{S1}(x_1) - n_2 \alpha_{22} g_2 S_2 B_{S2}(x_2) \right] . \tag{8b}$$

The equations can be rewritten in the slightly more convenient form

$$n_1 \alpha_{11} g_1 S_1 B_{S1}(x_1) - n_2 \alpha_{12} g_2 S_2 B_{S2}(x_2) - (kT/\mu_B^2 g_1 S_1) x_1 = 0 \tag{9a}$$

$$-n_1 \alpha_{12} g_1 S_1 B_{S1}(x_1) + n_2 \alpha_{22} g_2 S_2 B_{S2}(x_2) - (kT/\mu_B^2 g_2 S_2) x_2 = 0. \tag{9b}$$

We are particularly interested in the case where all the α_{ij} are negative and α_{12} has a considerably larger magnitude than α_{11} or α_{22}. Under these conditions, Eq. (9a) defines x_1 as an implicit function of x_2 which is continuous and positive for all positive values of x_2. Its derivative is

$$\frac{dx_1}{dx_2} = \frac{-n_2 \alpha_{12} g_2 S_2 B'_{S2}(x_2)}{(kT/\mu_B^2 g_1 S_1) - n_1 \alpha_{11} g_1 S_1 B'_{S1}(x_1)} , \tag{10}$$

where $B'_S(x)$ denotes $(d/dx)B_S(x)$. For α_{11} and α_{12} negative this expression is positive and finite for all values of x_2 provided either T is greater than absolute zero or α_{11} is not equal to zero. At $x = 0$, $B'_S(x) = (S+1)/3S$, so that

$$\left. \frac{dx_1}{dx_2} \right|_{x_2=0} = \frac{-n_2 \alpha_{12} g_2 (S_2 + 1)/3}{(kT/\mu_B^2 g_1 S_1) - n_1 \alpha_{11} g_1 (S_1 + 1)/3} . \tag{11}$$

This expression approaches zero as T becomes very large, and has the value

$$\frac{n_2 \alpha_{12} g_2 (S_2 + 1)}{n_1 \alpha_{11} g_1 (S_1 + 1)}$$

at $T = 0$.

By a similar argument, Eq. (9b) defines x_2 as an implicit function of x_1 for all the same conditions. It follows that, provided $(\alpha_{12}/\alpha_{11}) > (\alpha_{22}/\alpha_{12})$, there must exist a non-zero solution to Eqs. (9) if T is not too large. It also follows that, for T sufficiently large, the only possible solution is $x_1 = x_2 = 0$. We may define the Curie temperature, T_c, as the least upper bound of values of T for which a nonzero solution exists. A necessary condition for this temperature is that the two curves defined by Eqs. (9) should be tangent at the origin, which implies that

$$\begin{vmatrix} n_1 \alpha_{11} g_1^2 S_1(S_1 + 1)/3 - \dfrac{kT_c}{\mu_B^2} & n_2 \alpha_{12} g_1 g_2 S_1(S_2 + 1)/3 \\ \\ n_1 \alpha_{12} g_2 g_1 S_2(S_1 + 1)/3 & n_2 \alpha_{22} g_2^2 S_2(S_2 + 1)/3 - \dfrac{kT_c}{\mu_B^2} \end{vmatrix} = 0 . \qquad (12)$$

The Curie temperature is usually an easily measured quantity, so it is convenient to express the other interactions in terms of it. To this end, let us define $\beta_1 = \alpha_{11}/\alpha_{12}$, $\beta_2 = \alpha_{22}/\alpha_{12}$; then we can rewrite Eq. (12)

$$\begin{vmatrix} n_1 \beta_1 g_1^2 S_1(S_1 + 1)/3 - kT_c/\mu_B^2 \alpha_{12} & n_2 g_1 g_2 S_1(S_2 + 1)/3 \\ \\ n_1 g_1 g_2 S_2(S_1 + 1)/3 & n_2 \beta_2 g_2^2 S_2(S_2 + 1)/3 - kT_c/\mu_B^2 \alpha_{12} \end{vmatrix} = 0 . \qquad (13)$$

Then

$$kT_c/\mu_B^2 \alpha_{12} = \frac{1}{6} \left(n_1 \beta_1 g_1^2 S_1(S_1 + 1) + n_2 \beta_2 g_2^2 S_2(S_2 + 1) - \left\{ \left[n_1 \beta_1 g_1^2 S_1(S_1 + 1) \right. \right. \right.$$
$$\left. \left. \left. - n_2 \beta_2 g_2^2 S_2(S_2 + 1) \right]^2 + 4 n_1 n_2 g_1^2 g_2^2 S_1 S_2(S_1 + 1)(S_2 + 1) \right\}^{1/2} \right) , \qquad (14)$$

where the minus sign is chosen in the quadratic formula since T_c must be positive but α_{12} is negative. If we denote the right-hand side of Eq. (14) by -G, we get

$$1/\alpha_{12} = - \frac{G \mu_B^2}{kT_c} \qquad (15)$$

and Eqs. (9) become

$$-n_1 \beta_1 g_1^2 S_1^2 B_{S1}(x_1) + n_2 g_1 g_2 S_1 S_2 B_{S2}(x_2) - GTx_1/T_c = 0 \qquad (16a)$$

$$n_1 g_1 g_2 S_1 S_2 B_{S1}(x_1) - n_2 \beta_2 g_2^2 S_2^2 B_{S2}(x_2) - GTx_2/T_c = 0 . \qquad (16b)$$

These equations can be solved by means of numerical techniques in a fairly straight-forward manner. First we choose a pair of values for x_1 and x_2 which are fairly certain to be larger than the final solution. Using this x_2 we solve Eq. (16a) for x_1, and using x_1 we solve equation (16b) for x_2. We compare the new values of x_1 and x_2 with the previous ones, and if both changes are less than a predetermined tolerance we have found the solution. If not, we find the lines tangent to the two curves at the two new points we have found, solve the equations of these lines for a new x_1 and x_2, and repeat the process, which will converge in most cases after a few iterations.

APPLICATION TO LITHIUM FERRITE

Rado and Folen (4) have treated special cases of molecular field calculations in two set systems in which both sets of ion sites are occupied by the ion Fe^{+++}, in which case $S_1 = S_2 = 5/2$, and $g_1 = g_2 = 2$. With these restrictions, Eqs. (16) reduce to

$$-n_1 \beta_1 B_{5/2}(x_1) + n_2 B_{5/2}(x_2) - GTx_1/T_c = 0 \qquad (17a)$$

$$n_1 B_{5/2}(x_1) - n_2 \beta_2 B_{5/2}(x_2) - GTx_2/T_c = 0 , \tag{17b}$$

where

$$G = -\frac{7}{30} \left\{ n_1 \beta_1 + n_2 \beta_2 - \left[(n_1 \beta_1 - n_2 \beta_2)^2 + 4n_1 n_2 \right]^{1/2} \right\} . \tag{18}$$

Rado and Folen used a manual technique to calculate the magnetization vs temperature curve for lithium ferrite, $LiFe_5O_8$. This substance crystallizes in the spinel structure, which is based on a framework of oxygens in an arrangement which is a small distortion of cubic close packing. The cations are distributed among the interstices, some in "tetrahedral" or "A" sites with fourfold coordination and some in "octahedral" or "B" sites with sixfold coordination. In lithium ferrite two of the five iron ions occupy A sites. The substance has two arrangements for occupancy of the B sites by the remaining ions, depending on the previous thermal history of the sample. If the sample is rapidly cooled from a high temperature, the remaining three iron ions and the lithium ion occupy the B sites at random. On the other hand, if the sample is slowly cooled, the lithium ions occupy a particular subset of B sites (5) in a manner which possesses long-range order. The numbers n_1 and n_2 do not depend, at least to a first approximation, on the degree of the B site ordering but depend only on the total proportion of magnetic ions in the two types of sites.

Rado and Folen were able to find values for the ratios β_1 and β_2 which gave excellent agreement between the observed and calculated curves of net magnetization vs temperature. Because the net magnetization is, however, a function of the difference between the magnetizations of the individual sites, there remains the possibility either that the solution is not unique or that the success of the molecular field method in this case was largely fortuitous and the magnetizations of the individual sites are not adequately accounted for. That this might be the case is suggested by some recent nuclear magnetic resonance work (6) in which the magnetizations of both sites appeared to be higher than predicted at temperatures near the Curie temperature. In an effort to determine the sensitivity of the magnetization vs temperature curves to changes in the values of the molecular field parameters, we have calculated the curves for the parameters given in Rado and Folen's paper, as well as for some other sets of parameters chosen so as to give the same value of the net magnetization at the temperature $0.75\,T_c$. The programs used for these calculations are described in the appendix. The procedure was to calculate the curves of the two individual site magnetizations and the net magnetization using the Rado and Folen parameters, $\beta_1 = 0.54$, $\beta_2 = 0.22$. Then a new value of β_1 was specified, and the computer, by standard numerical methods determined the value of β_2 which gave the same net magnetization at $T = 0.75\,T_c$. Finally the computer calculated new curves of magnetization vs temperature. Curves were calculated for $\beta_1 = +0.20$ and for $\beta_1 = -0.45$. The latter curves were obtained as a result of an inadvertent error in coding the problem for the computer, but the results were highly instructive. Although this corresponds to a positive value for a_{11}, in which case a solution has not been previously shown to exist, the solution actually does exist, and in fact the curve differs from the original by only a few percent. Figure 1 shows the net magnetization as a function of temperature for the three pairs of values $\beta_1 = 0.54$, $\beta_2 = 0.22$; $\beta_1 = 0.20$, $\beta_2 = -0.0009$; and $\beta_1 = -0.45$, $\beta_2 = -0.42$. Figure 2 shows these values of β_2 plotted against β_1, and shows that there is a very nearly linear relationship between these parameters under the assumed system of constraints. The similarity of the curves of Fig. 1 is evidence that the parameters β_1 and β_2 are very strongly correlated, and that measurement of the magnetization curves is not a very sensitive measure of the values of these molecular field parameters.

Table 1 shows the A-site magnetizations alone, for the two extreme pairs of parameters. These curves are evidently also insensitive to the molecular field parameters, so that if a current neutron diffraction investigation confirms the nuclear magnetic resonance curves, it will be evidence that the agreement of the net magnetization data is
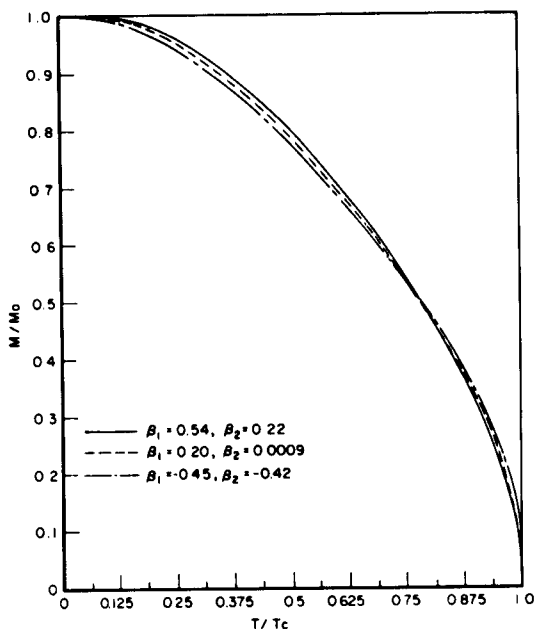
Fig. 1 - Net magnetization vs temperature curves for lithium ferrite for various possible values of the ratios of the molecular field coefficients

Fig. 2 - Plot of the ratio β_2 against the ratio β_1 for a constant value of net magnetization at $T = 0.75$ T_c. Magnetic measurements can be expected to locate the position of this line quite precisely, but the location of the best point on the line is very uncertainly determined.
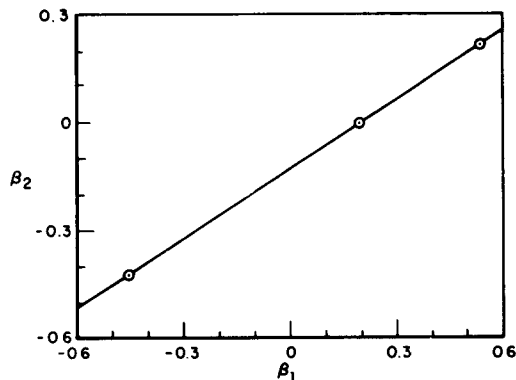
largely fortuitous, and that the molecular field approximation is inadequate in this degree of precision.

PROCEDURE IN CASES OF MORE THAN TWO ION SETS

In cases in which the magnetic structure includes more than two sets of magnetic ions, the possible structure types are much more numerous, and the mathematical treatment becomes correspondingly more complex. In some instances one of the interactions dominates all the others, and the equations can be solved in a manner similar to the one used for the simple two-set case. In order to eliminate the dominant interaction parameter in terms of the Curie temperature, it is necessary to solve an equation similar to Eq. (12) but of degree n, where n is the number of independent equations. This is likely to be difficult except in special cases, but it does have the advantage of including the reduced temperature, T/T_c, as a parameter in the equations. Thus the scale of the interaction strengths is fixed by the relatively precise measurement of the Curie temperature, and the shapes of the curves need only be used to determine ratios.

Table 1
Values of the Predicted A-Site Magnetization as a Function
of Temperature for Various Values of the Molecular Field
Coefficients

T/T$_c$	M_A/M_0		
	$\beta_1 = 0.54,$ $\beta_2 = 0.22$	$\beta_1 = 0.20,$ $\beta_2 = -0.0009$	$\beta_1 = -0.45,$ $\beta_2 = -0.42$
0.0625	1.000	1.000	1.000
0.1250	1.000	1.000	1.000
0.1875	0.998	0.998	0.997
0.2500	0.992	0.991	0.990
0.3125	0.980	0.978	0.977
0.3750	0.962	0.960	0.958
0.4375	0.939	0.937	0.934
0.5000	0.909	0.907	0.905
0.5625	0.873	0.872	0.870
0.6250	0.830	0.829	0.827
0.6875	0.777	0.776	0.775
0.7500	0.712	0.712	0.712
0.8125	0.632	0.632	0.633
0.8750	0.528	0.529	0.530
0.9375	0.382	0.383	0.385

In more complex cases, particularly where several of the interactions have similar magnitudes, so as to produce structures containing canted spins, there is no alternative to a direct attempt to find solutions to Eqs. (7). The starting point is the structure at absolute zero, as determined from magnetic and neutron diffraction measurements. At absolute zero the arguments of all Brillouin functions become infinite, with the values of the functions approaching unity. The value of a given Brillouin function at a lower temperature can be used as a first approximation at a higher temperature, while better approximations can be found by numerical techniques. In this method the predicted Curie temperature must be found by a numerical determination of the highest temperature at which a nonzero solution exists. It is a serious disadvantage of this procedure that the independent variable is absolute temperature rather than the reduced temperature, T/T$_c$. Thus, in order to fit experimental curves it is necessary to calculate the entire curve before adjusting the constants to correct the scale in such a way as to cause the solutions to vanish at the correct Curie temperature.

It is probable that each individual problem will have to be considered on its own merits. Many of the more complex systems are three-set systems with antiparallel alignments, such as the inverted ferrites of iron, cobalt, and nickel, and gadolinium-iron garnet. These would involve the solution of a cubic equation, which can be handled by analytic methods, although it is not easy to see in advance what the best procedure is going to be.

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Appendix A

PROGRAM TO CALCULATE MAGNETIZATION CURVES

The program used to calculate the curves of magnetization vs temperature for lithium ferrite is on NAREC tape 4658. This program can be used for magnetization calculation in any compound in which there are two sets of magnetic ions, and all magnetic ions have the same magnetic moment. With some simple changes the routine could be used where the magnetic moments on the two sites are different. The program contains within it a subroutine which calculates the value of the Brillouin function, $B_S(x)$, and its derivative, $B'_S(x)$, for values of S from 1/2 to 9/2 and for values of x up to 1000. It also contains a subroutine which solves the equation $pB_S(y) + qB_S(x) - ry = 0$ for y, given a value of x. Tape 4658 occupies NAREC locations 3ca0-3d5f, and it requires the fixed-point subroutine tape 4400-3d70 in locations 3d70-3fff. Locations 3d60-3d6f are used as working locations. We shall describe the individual parts of the program in detail.

EVALUATION OF THE BRILLOUIN FUNCTION

The Brillouin function, $B_S(x)$, is given in Eq. (4) in a form which is commonly written because of compactness, rather than for convenience of computation. For computation purposes it may be rewritten in the form

$$B_S(x) = \frac{(2S+1)\left[1 + e^{-(2S+1)x/S}\right](1 - e^{-x/S}) - (1 + e^{-x/S})\left[1 - e^{-(2S+1)x/S}\right]}{2S\left[1 - e^{-(2S+1)x/S}\right](1 - e^{-x/S})},$$

which is less compact, but which requires only the evaluation of two exponentials in addition to simple arithmetic operations. Similarly, the derivative $B'_S(x)$ takes the form

$$B'_S(x) = \frac{-(2S+1)^2 e^{-(2S+1)x/S}(1 - e^{-x/S})^2 + e^{-x/S}\left[1 - e^{-(2S+1)x/S}\right]^2}{S^2\left[1 - e^{-(2S+1)x/S}\right]^2(1 - e^{-x/S})^2},$$

which is a simple function of the same two exponentials. At x = 0 both of these formulas produce indeterminate forms, but a straightforward, although tedious, application of L'Hospital's rule gives the results $B_S(0) = 0$ and $B'_S(0) = (S+1)/3S$.

In order to keep all quantities within the range of values permitted in fixed point arithmetic on the NAREC, the argument of the Brillouin function is scaled by 1000 (decimal). The quantity 2S must be placed in the left address position of the first subroutine entry word. Since 9/2 is the largest acceptable value of S, it is immaterial whether decimal or hexadecimal notation is being considered by the programmer. The subroutine entry form is

$$s)\quad (2S)<XU>\quad woU$$

$$s+1)\quad s+1\ A\quad L03d20(3d42)\,.$$

Control will be returned to L0s + 2. If the entry is L03d20, $B_S(x)$ will be in the A register on return. If the entry is L03d42, $B_S(x)$ will be in the A register and $B'_S(x)$ will be in the U register on return.

SOLUTION OF INDIVIDUAL EQUATIONS

The equation $pB_s(y) + qB_s(x) - ry = 0$ defines y as an implicit function of x for all nonnegative values of x. A routine which solves for y as a function of x obviously will provide solutions of Eqs. (17a) and (17b) individually, given in each case an initial value for the independent variable. We use here the Newton-Raphson iterative method, whereby the second guess y_2 is obtained from the first guess y_1 by

$$y_2 = y_1 - \frac{pB_s(y_1) + qB_s(x) - ry_1}{pB'_s(y_1) - r} \ .$$

A third guess is obtained from the second, and so forth, until the equation is satisfied within a specified tolerance. When the proper value of y has been found, the derivative is computed from the relation

$$\frac{dy}{dx} = \frac{qB'_s(y)}{r - pB'_s(x)} \ .$$

The subroutine requires five parameters:

$$P_0 = p \times 10^{-2},$$

$$P_1 = q \times 10^{-2},$$

$$P_2 = r \times 10^{-2},$$

$$P_3 = 2S \text{ in the left address position},$$

$$P_4 = x \times 10^{-3}.$$

These are stored in consecutive locations, the location of P_0 being supplied to the subroutine in the entry. The entry form is

```
        s)      (address of P0)<XU>      sU

    s + 1)              s + 1 A          L03d00 .
```

On completion the control is returned to $L0s+2$ with $10^{-3} y$ in the A register and 10^{-2} dy/dx in the U register.

SIMULTANEOUS SOLUTION OF MOLECULAR FIELD EQUATIONS

The main subroutine makes use of the two previous subroutines to solve simultaneously the two equations

$$-n_1\beta_1 B_s(x) + n_2 B_s(y) - GTx/T_c = 0$$

$$n_1 B_s(x) - n_2\beta_2 B_s(y) - GTy/T_c = 0 ,$$

where

$$G = -\left\{ n_1\beta_1 + n_2\beta_2 - \left[(n_1\beta_1 - n_2\beta_2)^2 + 4n_1 n_2 \right]^{1/2} \right\} (J+1)/6J .$$

Starting from an initial guess (x_0, y_0) the point (x_1, y_0) is found by solving the first equation, and the coefficients of the line

$$\frac{x - x_1}{y - y_0} = \frac{dx}{dy} (x_1, y_0)$$

are determined. Similarly, the point (x_0, y_1) is found by solving the second equation, and the coefficients of the line

$$\frac{y - y_1}{x - x_0} = \frac{dy}{dx} (x_0, y_1)$$

are determined. Finally the intersection of these two lines is taken as the next guess, and the process is repeated until the differences in the x and y coordinates of two successive guesses are less than the specified tolerances.

The subroutine requires six parameters:

$$P_0 = -\beta_1, \text{ with } \beta_1 < 1,$$

$$P_1 = -\beta_2, \text{ with } \beta_2 < 1,$$

$$P_2 = n_1 \times 10^{-2},$$

$$P_3 = n_2 \times 10^{-2},$$

$$P_4 = 2S \text{ in the left address position},$$

$$P_5 = T/T_c.$$

The entry form is

s)   (address of P_0)<XU>   sU

s + 1)   s + 1 A   LO3ca0 .

The routine returns to the main program at $LOs + 2$ with $B_s(y)$ in the A register and $B_s(x)$ in the U register.

*   *   *

dominant one. A computation of the shapes of the curves of the magnetization as a function of temperature shows that, while magnetic and neutron diffraction measurements can determine quite precisely the value of a linear function of these fractions, the actual values of the individual fractions are less precisely determined. It follows that any experimental deviation from the calculated curves is due to an inadequacy of the theory rather than to incorrect values of the parameters. Finally, methods of attack for computation of more complex cases are discussed.